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                 introduction of free HIT display format
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                 records back to 1992
                CAS REGISTRY Source of Registration (SR) searching
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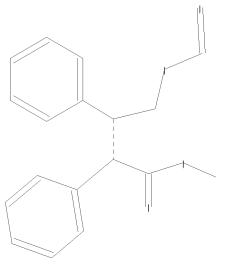
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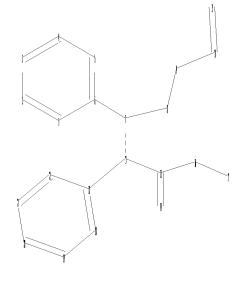
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chain nodes :

7 8 9 10 11 13 14 15 16 17

ring nodes :

1 2 3 4 5 6 12 18 19 20 21 22

chain bonds :

6-7 7-8 7-11 8-9 9-10 10-15 11-12 11-13 13-14 13-16 16-17

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-18 \quad 12-22 \quad 18-19 \quad 19-20 \quad 20-21 \quad 21-22$ 

exact/norm bonds :

7-11 8-9 9-10 10-15 13-14 13-16 16-17

exact bonds :

6-7 7-8 11-12 11-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22

isolated ring systems : containing 1 : 12 :

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom

## L1 STRUCTURE UPLOADED

=> s sam sss 11

SAMPLE SEARCH INITIATED 10:55:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 257 TO 903 PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> d sca

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)$ 

MF C40 H38 F2 O10 S2 . Na

Na

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-$ 

MF C40 H38 F2 O10 S2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-bis(nitrooxy)pentyl]oxy]-1-[4-bis(nitrooxy)pe$ 

(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, ( $\alpha Z$ )-

MF C25 H28 N2 O13 S

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (2)- (9CI)

MF C24 H21 N O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s full sss 11
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 11:12:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 767 TO ITERATE

100.0% PROCESSED 767 ITERATIONS 84 ANSWERS

SEARCH TIME: 00.00.01

L3 84 SEA SSS FUL L1

=> d sca

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-

MF C24 H28 F2 N O6 S

CI COM

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, ( $\alpha$ Z)-

MF C25 H30 O7 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, <math>(\alpha Z)$ -

MF C29 H38 N2 O9 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-4-[[(2R)-1-oxo-2-propyloctyl]oxy]-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)

MF C33 H46 F2 N O6 S . Br

Absolute stereochemistry. Double bond geometry as shown.

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, ( $\alpha$ Z)-

MF C24 H26 N2 O12 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4- (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, ( $\alpha$ Z)-MF C25 H29 N O9 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester, ( $\alpha$ Z)-

MF C28 H31 F N2 O9 S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester

MF C23 H23 F2 N O8 S

Absolute stereochemistry. Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha = [2 - (acetyloxy) - 1 - [4 - (methylsulfonyl)phenyl]ethylidene] -, 3 - (arboxy - 2 - [4 - (methylsulfonyl)phenyl] - 3 - phenyl$ 

3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester

MF C36 H32 O10 S2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)-

MF C23 H25 Br O7 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(benzoyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)

MF C25 H22 O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
- MF C24 H29 F N O6 S . Br

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester

MF C30 H38 N2 O11 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, <math>(\alpha Z)-(\alpha Z)$ 

MF C26 H31 N O10 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluoropheny1)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl]oxy]-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-

MF C36 H42 F2 N O8 S

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, ( $\alpha$ Z)-

MF C25 H28 N2 O12 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[3-(bromomethyl)benzoyl]oxy]-1-[4-$ 

(methylsulfonyl)phenyl]ethylidene]-, methyl ester,  $(\alpha Z)$ -

MF C26 H23 Br O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-2-methyl-1-[4-

(methylsulfonyl)phenyl]propylidene]-3-fluoro-, methyl ester, ( $\alpha Z$ )-

MF C22 H23 F O6 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, ( $\alpha$ Z)-,

(2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1)

MF  $C24 H25 F2 N O8 S \cdot C2 H F3 O2$ 

CM 1

Absolute stereochemistry. Double bond geometry as shown.

CM 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

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ΙN Benzeneacetic acid,  $\alpha-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-$ 3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-[4-methylsulfonyl]-1-[4-methylsulfonyl]-1-[4-methylsulfonyl]-1-[4-m(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)

C40 H38 F2 O10 S2 . Na MF

Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

ΙN Benzeneacetic acid,  $\alpha$ -[2-[[3-[[(1,1dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)-C32 H38 O7 S Si MF

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)

MF C20 H20 O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,

(2S)-2-amino-3-ethoxy-3-oxopropyl ester

MF C24 H25 F2 N O8 S

Absolute stereochemistry. Double bond geometry unknown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2-buten-1-yl ester

MF C30 H38 Br N O8 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-MF C25 H29 N O10 S

Double bond geometry as shown.

$$\begin{array}{c|c} O & O & (CH_2) & O & NO_2 \\ \hline & O & & & \\ \hline & O & & \\ \hline &$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1H-Benzimidazole-4-carboxylic acid,

1H-Benzimidazole-4-carboxylic acid, 2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl ester

MF C43 H36 F2 N6 O7 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, ( $\alpha$ Z)-

MF C25 H28 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ E)-MF C32 H38 O7 S Si

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) MF C19 H18 F N O6 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, ( $\alpha$ Z)-

MF C24 H25 F2 N O8 S

CI COM

Absolute stereochemistry. Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester, sodium salt (1:1)
- MF C36 H32 O10 S2 . Na

Na

# HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[3-[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester,  $(\alpha Z)$ -

MF C26 H23 N O10 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenepropanoic acid,  $\beta\text{-}[(1\text{-}oxopropoxy)\text{methyl}]\text{-}\alpha\text{-}phenyl\text{-}, ethyl ester}$ 

MF C21 H24 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)

MF C24 H28 F2 N O6 S . Br

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester,  $(\alpha Z)$ -

MF C25 H29 Br O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, ( $\alpha$ Z)-

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Double bond geometry as shown.

PAGE 1-A

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, ( $\alpha$ Z)-MF C28 H26 N2 O13 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)-

MF C26 H23 Br O7 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) MF C19 H17 F2 N O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluoro

Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-

MF C24 H29 F N O6 S

CI COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid,  $\alpha$ -[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
- MF C36 H28 F4 O10 S2
- CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl

ester, hydrochloride (1:1), ( $\alpha Z$ )-MF C29 H38 N2 O10 S . C1 H

Double bond geometry as shown.

● HCl

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid,  $\alpha-[2-[4-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, <math>(\alpha Z)$ -
- MF C44 H44 F2 O12 S2
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI) MF C25 H30 F2 N2 O6 S

Absolute stereochemistry. Double bond geometry unknown.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester

MF C25 H30 N2 O9 S

CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, methyl ester, <math>(\alpha Z)-$  MF C24 H27 N O9 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-ethoxy-3-oxopropyl ester, ( $\alpha$ Z)- MF C29 H33 F2 N O10 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, ( $\alpha$ Z)-

MF C23 H24 N2 O13 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)-

MF C26 H24 O8 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(aminosulfonyl)phenyl]-2-

(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)

MF C24 H21 N O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-

MF C24 H28 F2 N O6 S

CI COM

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, 3-(3,4-difluorophenyl)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-[4-(methylsulfonyl)phenyl]-2-buten-1-yl ester

MF C42 H44 F4 O9 S2 Si

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-MF C24 H27 N O10 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C44 H44 F2 O12 S2 . Na

Double bond geometry as shown.

● Na

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[(2S)-2-amino-3-hydroxy-1-oxopropoxy]-1-[4- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI) MF C22 H23 F2 N O7 S

Absolute stereochemistry. Double bond geometry unknown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4- (methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, ( $\alpha$ Z)-MF C26 H31 N O9 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-

Double bond geometry as shown.

$$\begin{array}{c|c} O & O & (CH_2) \stackrel{1}{\cancel{4}} & NO_2 \\ \hline O & O & \\ \hline Z & OMe & \\ \hline Me & Ph & \\ \hline \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)

MF C24 H29 F N O6 S . Br

Double bond geometry as shown.

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[[4,5-

bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, ( $\alpha$ Z)-MF C25 H28 N2 O13 S

Double bond geometry as shown.

$$\begin{array}{c} O_2N \\ O \\ O \\ CH_2)_3 \end{array} \begin{array}{c} O \\ NO_2 \\ O \\ O \\ O \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid,  $\alpha$ -[2-[[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester,  $(\alpha Z)$ -MF C32 H38 O8 S Si

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(aminosulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)

MF C19 H19 N O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester,

Double bond geometry as shown.

Me S Ph 
$$Z$$
 Ph  $Z$  O  $CH_2)_6$  O  $Z$  OAc

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[4-(acetyloxy)-2-(3,4-difluoropheny1)-3-[4-(methylsulfony1)pheny1]-1-oxo-2-buten-1-y1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-3,4-difluoro-, sodium salt (1:1)$ 

MF C36 H28 F4 O10 S2 . Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, ( $\alpha$ Z)-

MF C26 H29 N O11 S

Absolute stereochemistry. Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-4-[[(2R)-1-oxo-2-propyloctyl]oxy]-2-buten-1-yl]oxy]-N,N,N-trimethyl-

MF C33 H46 F2 N O6 S

CI COM

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN L-Aspartic acid, 4-[3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester

MF C23 H23 F2 N O8 S

Absolute stereochemistry. Double bond geometry unknown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, ( $\alpha Z$ )-MF C24 H27 N O9 S

Double bond geometry as shown.

$$AcO$$
 $CH_2)_5$ 
 $NO_2$ 
 $Me$ 
 $Ph$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[3-[(nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-MF C26 H23 N O9 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
- MF C24 H28 F2 N O6 S . Br

Double bond geometry as shown.

● Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)-MF C24 H26 N2 O13 S

Double bond geometry as shown.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, <math>(\alpha Z)$ -

MF C26 H31 Br O7 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI)

MF C20 H19 F O6 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-

MF C24 H29 F N O6 S CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethylester, <math>(\alpha Z)$ -

MF C29 H38 N2 O10 S

CI COM

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (<math>\alpha$ Z)-

MF C30 H37 N O11 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, 3,4-difluoro- $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[(2R)-1-oxo-2-propyloctyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-

MF C29 H36 F2 O6 S

Absolute stereochemistry.

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, ( $\alpha$ Z)-

MF C23 H24 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI)

MF C25 H30 N2 O9 S . Cl H

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester,  $(\alpha Z)$ -

MF C27 H31 F N2 O7 S2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, ( $\alpha$ E)- (9CI)

MF C25 H30 F2 N2 O6 S

Absolute stereochemistry. Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-$ 

3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-C40 H38 F2 O10 S2 COM

MF CI

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid,  $\alpha$ -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, ( $\alpha$ Z)-MF C24 H27 Br O7 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) MF C20 H18 F2 O6 S

ALL ANSWERS HAVE BEEN SCANNED

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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 201.24 201.46

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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

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E1 THROUGH E34 ASSIGNED

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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 5.90 207.36

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=> s 13 and 15 L6 4 L3 AND L5

=> d sca

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, ( $\alpha$ Z)-

MF C24 H26 N2 O12 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, ( $\alpha$ Z)-

MF C23 H24 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, ( $\alpha$ Z)-

MF C25 H28 N2 O12 S

Double bond geometry as shown.

$$AcO$$
 $CH_2)_4$ 
 $NO_2$ 
 $NO_2$ 

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, ( $\alpha$ Z)-

MF C25 H28 N2 O12 S

Absolute stereochemistry. Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file zcaplus\

'ZCAPLUS\' IS NOT A VALID FILE NAME

SESSION CONTINUES IN FILE 'REGISTRY'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file zcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.40 209.76

FULL ESTIMATED COST

FILE 'ZCAPLUS' ENTERED AT 11:18:58 ON 17 JUN 2009
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FILE COVERS 1907 - 17 Jun 2009 VOL 150 ISS 25
FILE LAST UPDATED: 15 Jun 2009 (20090615/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L7 18 L3

=> s 17 and (nitrosated or nitrosylated)

1340 NITROSATED

604 NITROSYLATED

L8 1 L7 AND (NITROSATED OR NITROSYLATED)

=> d sca

L8 1 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN

IC ICM A61K031-40

ICS A61K031-415; A61K031-421; A61K031-50; C07D207-325; C07D231-06; C07D237-14; C07D263-04; C07D263-06

CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 1

TI Preparation of nitrosated and nitrosylated

```
ST
    cyclooxygenase 2 inhibitor nitrosated nitrosylated
    prepn
    Analgesics
IΤ
    Anti-inflammatory agents
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ΙT
    Nitroso compounds
    Nitrosvl complexes
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ΙT
    329900-75-6, cyclooxygenase-2
    RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (mediated disorders; treatment; preparation of nitrosated and
        nitrosylated cyclooxygenase-2 inhibitors)
ΤТ
    205580-05-8P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
                  346683-70-3P
ΤТ
    346683-69-0P
                                  346683-71-4P
                                                 346683-72-5P
                                                                346683-73-6P
    346683-75-8P
                   346683-76-9P
                                  346683-77-0P
                                                 346683-78-1P
                                                                346683-79-2P
    346683-80-5P 346683-81-6P 346683-82-7P 346683-83-8P
    346683-84-9P
                   346683-85-0P
                                 346683-86-1P
                                                346683-87-2P
                                                                346683-88-3P
    347162-90-7P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ΙT
    346683-99-6P
                   346684-20-6P
                                  346684-22-8P
    RL: BYP (Byproduct); PREP (Preparation)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ΙT
     52-67-5, D-Penicillamine
                                53-86-1, Indomethacin
                                                       78-83-1,
    2-Methyl-1-propanol, reactions 78-94-4, Methyl vinyl ketone, reactions
    100-53-8, Benzyl mercaptan 627-18-9, 3-Bromo-1-propanol
                                                                1445-73-4,
    1-Methyl-4-piperidone
                           1778-09-2, 4-Methylthioacetophenone
                                                                  2417-72-3,
                                  3446-89-7, 4-Methylthiobenzaldehyde
    Methyl 4-bromomethylbenzoate
    18162-48-6, tert-Butyldimethylsilyl chloride
                                                  21382-98-9,
                               24214-73-1, Cyclohexylhydrazine hydrochloride
     4-Methylthiobenzonitrile
    32047-53-3, 1-Amino-2-methyl-2-propanethiol hydrochloride 61040-78-6,
    2,4,6-Trimethoxybenzyl alcohol 90878-19-6, Phenethylmagnesium chloride
    194596-99-1
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
                  28399-82-8P
                                40027-88-1P
                                              73303-88-5P,
ΤТ
    15581-80-3P
                                     86864-60-0P
                                                   89031-84-5P
                                                                 136881-95-3P
     2-Methyl-2-mercapto-1-propanol
    157672-00-9P
                   170571-19-4P
                                 170571-20-7P
                                                 170571-71-8P
                                                                179174-91-5P
    179174-92-6P
                   179174-93-7P
                                  179174-94-8P
                                                 181695-72-7P
                                                                181695-81-8P
    189501-33-5P
                  189501-34-6P
                                  205579-90-4P
                                                 213763-90-7P
                                                                213764-17-1P
    215124-07-5P 215124-20-2P
                                  291518-72-4P
                                                 346683-89-4P
                                                                346683-90-7P
    346683-91-8P
                   346683-92-9P
                                  346683-94-1P
                                                 346683-95-2P
                                                                346683-96-3P
    346683-97-4P 346683-98-5P 346684-00-2P
                                                 346684-01-3P
                                                                346684-02-4P
    346684-03-5P 346684-04-6P 346684-05-7P 346684-06-8P
                                                                346684-07-9P
```

cyclooxygenase-2 inhibitors

```
346684-08-0P 346684-09-1P 346684-10-4P 346684-11-5P
                                                                 346684-12-6P
     346684-13-7P
                    346684-14-8P 346684-15-9P 346684-19-3P 346684-21-7P
                                                  346684-16-0P
                                                                 346684-17-1P
                                                  347162-91-8P
     346684-18-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ΤТ
     346684-23-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ALL ANSWERS HAVE BEEN SCANNED
=> s 17 and (nitrosated or nitrosylated or NO or (nitric (w) oxide))
          1340 NITROSATED
           604 NITROSYLATED
       3932570 NO
        220094 NOS
          2032 NOES
       4060112 NO
                 (NO OR NOS OR NOES)
        223122 NITRIC
             3 NITRICS
        223125 NITRIC
                 (NITRIC OR NITRICS)
       1991269 OXIDE
        377613 OXIDES
       2097881 OXIDE
                 (OXIDE OR OXIDES)
        131578 NITRIC (W) OXIDE
T.9
           11 L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE))
=> d sca
                 ZCAPLUS COPYRIGHT 2009 ACS on STN
L9
     11 ANSWERS
     ICM C07C317-24
     ICS A61K031-21
INCL 514509000; 558482000
     25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
CC
     Section cross-reference(s): 1
TΙ
     Process for making nitric oxide releasing prodrugs of
     diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors
    nitric oxide releasing prodrug diphenylbutenoate hexyl
ST
    nitrate
ΤТ
     Drug delivery systems
        (prodrugs; preparation of nitric oxide releasing
        prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
ΙT
     329900-75-6, Cyclooxygenase 2
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; preparation of nitric oxide releasing
        prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     10102-43-9, Nitric oxide, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
ΤТ
     64-19-7, Acetic acid, uses 67-68-5, Dmso, uses 68-12-2, Dmf, uses
     75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 75-52-5,
                        127-19-5, N,N-Dimethylacetamide
                                                           872-50-4,
     Nitromethane, uses
     1-Methyl-2-pyrrolidinone, uses 1300-21-6, Dichloroethane 25321-22-6,
     Dichlorobenzene
```

```
RL: NUU (Other use, unclassified); USES (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     937-14-4, m-Chloroperbenzoic acid
                                         1504-58-1, 3-Phenyl-2-propyn-1-ol
ΙT
     4286-55-9
               7722-84-1, Hydrogen peroxide, reactions 10058-23-8,
     Potassium peroxymonosulfate
                                  11138-47-9, Sodium perborate
                                                                   74087-85-7,
     Dimethyldioxirane
                        78948-87-5, Magnesium monoperoxyphthalate
     210292-04-9, 4-Methylthiophenylmagnesium chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     176594-44-8P
                    179174-79-9P
                                  754242-10-9P 754242-11-0P
     754242-12-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     754241-98-0P
ΤТ
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
=> d ibib hitstr 1-11
THE ESTIMATED COST FOR THIS REQUEST IS 42.79 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) / N: y
     ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
                         2008:465556 ZCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         148:523285
TITLE:
                         Development of a discriminating in vitro dissolution
                         method for a poorly soluble NO-donating
                         selective cyclooxygenase-2 inhibitor
AUTHOR(S):
                         Papp, Robert; Luk, Pauline; Mullett, Wayne M.; Kwong,
                         Elizabeth; Debnath, Smita; Thibert, Roch
CORPORATE SOURCE:
                         Drug Metabolism and Pharmacokinetics, Merck Frosst
                         Center for Therapeutic Research, Kirkland, QC, H9H
                         3L1, Can.
SOURCE:
                         Journal of Pharmaceutical and Biomedical Analysis
                         (2008), 47(1), 16-22
                         CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER:
                         Elsevier B.V.
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
ΙT
     754241-98-0
     RL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (development of discriminating in vitro dissoln. method for poorly soluble
        NO-donating cyclooxygenase-2 inhibitor)
RN
     754241-98-0 ZCAPLUS
     Benzeneacetic acid, \alpha-[2-(acetyloxy)-1-[4-
CN
     (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (<math>\alpha Z)-
     (CA INDEX NAME)
```

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:495882 ZCAPLUS

DOCUMENT NUMBER: 145:14695

TITLE: Compounds for targeting mechanisms implicated in the

progression of stroke

INVENTOR(S): Munoz, Benito; Payne, Joseph E.; Prasit, Petpiboon;

Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas

APPLICATION NO.

DATE

S.; McGuire, Angela R.

DATE

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 63 pp.

CODEN: PIXXD2

KIND

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.

WO 200									WO 2	005-	JS40	851		2	0051	110
WO 200	060554	0.4		А3		2006	0810									
W	AE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,
	KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
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PAGE 1-B

IT 887908-54-5 887908-56-7
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (compds. for targeting mechanisms implicated in progression of stroke)
RN 887908-54-5 ZCAPLUS
CN 1H-Benzimidazole-4-carboxylic acid,
 2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-,

2-ethoxy-1-[[2'-(2H-tetrazol-5-y1)[1,1'-bipheny1]-4-y1]methy1]-, (2Z)-3-(3,4-difluoropheny1)-4-ethoxy-2-[4-(methylsulfony1)pheny1]-4-oxo-2-buten-1-yl ester (CA INDEX NAME)

RN 887908-56-7 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl]oxy]-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:383478 ZCAPLUS

DOCUMENT NUMBER: 144:432558

TITLE: Preparation of methylsulfonylphenylalkenoates as water

soluble prodrugs of COX-2 inhibitors.

INVENTOR(S): Munoz, Benito; Payne, Joseph Edward; Prasit,

Petpiboon; Reger, Thomas S.; Smith, Nicholas D.;

Stock, Nicholas S.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.									APPLICATION NO.								
		A1 20060427									007							
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	ВG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	ΚM,	KΡ,	KR,	KZ,	
		LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	
		NA,	NG,	ΝI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	
		SK,	SL,	SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	
		YU,	ZA,	ZM,	ZW													
	RW	: AT,																
							MC,											
			•			•	GN,			•				•			•	
							NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,	AZ,	BY,	
			KZ,												_			
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ΙΤ	885020						8502	0-36	-0P									
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RN	prc 885020	drugs -33-7				nibl	cors	,										

Ethanaminium, 2-[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-

(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA

Double bond geometry as shown.

INDEX NAME)

CN

RN 885020-34-8 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

RN 885020-36-0 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, ( $\alpha$ Z)-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 885020-35-9

C24 H25 F2 N O8 S CMF

Absolute stereochemistry. Double bond geometry as shown.

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 885020-37-1 ZCAPLUS

CN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-4](methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester (CA INDEX NAME) Absolute stereochemistry. Double bond geometry as shown.

RN 885020-38-2 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, ( $\alpha$ E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 885020-42-8P 885020-43-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)

RN 885020-42-8 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1) (CA INDEX NAME)

• Br-

RN 885020-43-9 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1) (CA INDEX NAME)

Double bond geometry as shown.

• Br-

IT 885020-47-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)

RN 885020-47-3 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-ethoxy-3-oxopropyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1315893 ZCAPLUS

DOCUMENT NUMBER: 144:212486

TITLE: Synthesis of a NO-Releasing Prodrug of

Rofecoxib

AUTHOR(S): Engelhardt, F. Conrad; Shi, Yao-Jun; Cowden, Cameron

J.; Conlon, David A.; Pipik, Brenda; Zhou, George;

McNamara, James M.; Dolling, Ulf-H.

CORPORATE SOURCE: Department of Process Research, Merck Company, Rahway,

NJ, 07065-0900, USA

SOURCE: Journal of Organic Chemistry (2006), 71(2), 480-491

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:212486

IT 875783-67-8P

RL: BYP (Byproduct); PREP (Preparation)

(synthesis of a NO-releasing prodrug of rofecoxib in five

chemical steps from 3-phenyl-2-propyn-1-ol)

RN 875783-67-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester,

 $(\alpha Z, \alpha'Z) - (9CI)$  (CA INDEX NAME)

Double bond geometry as shown.

Me 
$$\frac{Q}{S}$$
  $\frac{Q}{S}$   $\frac$ 

IT 754242-04-1P

RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation) (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)

RN 754242-04-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, ( $\alpha Z$ )- (CA INDEX NAME)

Double bond geometry as shown.

IT 754242-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)

RN 754242-12-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

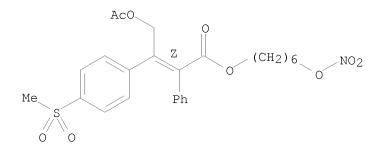
Double bond geometry as shown.

IT 754241-98-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)

RN 754241-98-0 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, ( $\alpha$ Z)-(CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:963804 ZCAPLUS

DOCUMENT NUMBER: 143:266677

TITLE: Process for making nitric oxide

releasing prodrugs of diary1-2-(5H)-furanones as

cyclooxygenase-2 inhibitors

INVENTOR(S): Shi, Yao-Jun; Engelhardt, F. Conrad; Cowden, Cameron

John; Conlon, David A.; Pipik, Brenda

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20050192346	A1	20050901	US 2005-66676		20050225
PRIORITY APPLN. INFO.:			US 2004-549126P	P	20040301
OTHER SOURCE(S).	CASBEZ	ОТ 143•2666	77. MARPAT 143.26667	7	

OTHER SOURCE(S): CASREACT 143:266677; MARPAT 143:266677

IT 754242-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 754242-12-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, ( $\alpha Z$ )-(CA INDEX NAME)

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 754241-98-0 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

Double bond geometry as shown.

L9 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:696873 ZCAPLUS

DOCUMENT NUMBER: 143:172624

TITLE: Preparation of nitric oxide

releasing prodrugs of diaryl-2(5H)-furanones as

cyclooxygenase-2 inhibitors

INVENTOR(S): Dufresne, Claude; Berthelette, Carl; Li, Lianhai;

Guay, Daniel; Gallant, Michel; Lacombe, Patrick; Aspiotis, Renee; Wang, Zhaoyin; Sturino, Claudio F.

PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	NO.	KIN	D	DATE			APPL		DATE							
WO 200	50708	83		A1	A1 20050804				WO 2	005-		20050125				
W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
RW	: BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,
	ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,
	RO,	SE,	SI,	SK,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,
	MR,	NΕ,	SN,	TD,	ΤG											
AU 200	52062	28		A1		2005	0804		AU 2	005-		20050125				
CA 255	4334			A1		2005	0804		CA 2	005-	2554.	334		2	0050	125
EP 171	1459			A1		2006	1018		EP 2	005-	7064	13		2	0050	125
R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
						RO,										
CN 191	4169			А		2007	0214		CN 2	005-	8000	3263		2	0050	125
JP 200	75204	83		Τ		2007	0726		JP 2	006-	5498	14		2	0050	125

US 20080242643 Α1 20081002 US 2006-586381 20060718 IN 2006-DN4347 IN 2006DN04347 20060727 Α 20070713 Р PRIORITY APPLN. INFO.: US 2004-539666P 20040127 WO 2005-CA83 W 20050125 CASREACT 143:172624; MARPAT 143:172624 OTHER SOURCE(S): 861430-33-3P 861430-34-4P 861430-36-6P 861430-38-8P RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of nitric oxide releasing prodrugs of diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors) RN 861430-33-3 ZCAPLUS CN Benzeneacetic acid,  $\alpha$ -[2-[[[[4,5bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 861430-34-4 ZCAPLUS CN Benzeneacetic acid,  $\alpha$ -[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester,  $(\alpha Z)$ - (CA INDEX NAME)

RN 861430-36-6 ZCAPLUS

CN Benzeneacetic acid,  $\alpha-[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, <math>(\alpha Z)-$  (CA INDEX NAME)

Double bond geometry as shown.

RN 861430-38-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:696865 ZCAPLUS

DOCUMENT NUMBER: 143:193802

TITLE: Preparation of nitric oxide

releasing prodrugs of diaryl-2(5H)-furanones as

cyclooxygenase-2 inhibitors

INVENTOR(S): Berthelette, Carl; Li, Lianhai; Beaulieu, Christian;

Wang, Zhaoyin; Sturino, Claudio F.

PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	ATENT	KIN	D	DATE		-	APPL	ICAT		DATE									
W(	2005	0708	 74		A1	_	2005	0804	WO 2005-CA84						20050125				
	W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,		
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NA,	NI,		
		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
		ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,		
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,		
		MR,	ΝE,	SN,	TD,	ΤG													
JA	J 2005	2062	29		A1		2005	0804		AU 2	005-	2062.	29		2	0050	125		
CA	A 2554	333			A1		2005	0804	1	CA 2	005-		20050125						
EI	2 1711	457			A1		2006	1018		EP 2	005-	7064	14		2	0050	125		
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,		
		ΙE,	SI,	LT,	LV,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	IS			
Cl	1 1914	151			Α		2007	0214	1	CN 2	005-	8000	3240		2	0050	125		
JI	2007	5204	84		Τ		2007	0726		JP 2	006-	5498	15		2	0050	125		
US	2008	0227						0918		US 2	006-	5865	73		2	0060	718		
11	1 2006	DN 0 4	343		А		2007	0713		IN 2	006-1	DN43	43		2	0060	727		
PRIORI	TY APP	LN.	INFO	.:						US 2	004-	5401	01P	]	P 21	0040	127		

OTHER SOURCE(S): CASREACT 143:193802; MARPAT 143:193802

IT 861655-83-6P 861655-84-7P 861655-85-8P

861655-86-9P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing prodrugs of diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 861655-83-6 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 861655-84-7 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 861655-85-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

RN 861655-86-9 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:739958 ZCAPLUS

DOCUMENT NUMBER: 141:260542

TITLE: Preparation of nitric oxide

releasing prodrugs of diaryl-2-(5H)-furanones as

selective cyclooxygenase-2 inhibitors

INVENTOR(S): Berthelette, Carl; Li, Lianhai; Sturino, Claudio;

Wang, Zhaoyin

PATENT ASSIGNEE(S): Merck Frosst Company, Can. SOURCE: U.S. Pat. Appl. Publ., 19 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	DATE			APPL	ICAT	DATE								
								_						
US 2004017633	040176331 A1						US 2	004-	2	20040301				
US 7169809		В2		2007	070130									
AU 2004240700	J 2004240700 A1						0041202 AU 2004-240700 200403							
CA 2517490	A 2517490 A1						CA 2	004-	2517	490		2	0040	301
WO 2004103955	)	A1		20041202 WO 2004-CA314 200						20040301				
W: AE, <i>P</i>	AG, AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
CN, C	CO, CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
GE, (	SH, GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
LK, I	LR, LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG EP 1601644 20051207 EP 2004-761562 20040301 Α1 EP 1601644 В1 20090527 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK JP 2007516954 20070628 JP 2006-529472 20040301 PRIORITY APPLN. INFO.: US 2003-452124P Ρ 20030305 WO 2004-CA314 W 20040301 OTHER SOURCE(S): MARPAT 141:260542 754241-98-0P 754241-99-1P 754242-00-7P 754242-01-8P 754242-02-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors) 754241-98-0 ZCAPLUS RN CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester,  $(\alpha Z)$ -(CA INDEX NAME)

Double bond geometry as shown.

RN 754241-99-1 ZCAPLUS

CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 754242-00-7 ZCAPLUS CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 754242-01-8 ZCAPLUS CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 754242-02-9 ZCAPLUS
CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

IT 754242-04-1P 754242-08-5P 754242-09-6P 754242-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

RN 754242-04-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4- (methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 754242-08-5 ZCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

RN 754242-09-6 ZCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.

RN 754242-12-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN T.9 2004:101124 ZCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 140:163574 TITLE: Preparation of nitric oxide releasing diary1-2-(5H)-furanone prodrugs as selective

cyclooxygenase-2 inhibitors for treatment inflammatory diseases

INVENTOR(S): Berthelette, Carl; Lachance, Nicholas; Li, Lianhai; Sturino, Claudio; Wang, Zhaoyin; Young, Robert N.;

Dufresne, Claude

CODEN: PIXXD2

PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

PCT Int. Appl., 129 pp. SOURCE:

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.					KIND		DATE		APPL	ICAT	DATE					
WO	2004011421			A1		20040205			WO 2	003-	20030724						
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KR,	KΖ,	LC,	LK,	LR,	LS,
		LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	ΝI,	NO,	NZ,	OM,	PG,
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ΤJ,	TM,	TN,	TR,
		TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW				
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FΙ,	FR,	GB,	GR,	HU,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
							CM,										
CA	CA 2493082								CA 2003-2493082								
AU	U 2003252515						AU 2003-252515										
EP	1527	1527045			A1 20050			0504		EP 2					2		
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
							RO,										
	2005									US 2	005-	5210	75		2	0050	112
	7199				В2		2007	0403									
CORIT	ORITY APPLN. INFO.:							US 2002-3986									
											002-					0021	
										–	003-				W 2	0030	724
	ER SOURCE(S):						T 14	0:16	3574	; MA	RPAT	140	:163	574			
	4069-																
RL	: BYP	(By	prod	uct)	; PR	EP (	Prep	arat.									

(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)

654069-14-4 ZCAPLUS RN

Benzeneacetic acid,  $\alpha$ -[2-[[3-[[(1,1-CN dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha E$ )- (CA INDEX NAME)

IT 654068-75-4P 654068-76-5P 654068-79-8P 654068-81-2P 654068-83-4P 654068-84-5P 654068-85-6P 654068-86-7P 654068-87-8P 654068-88-9P 654068-89-0P 654068-90-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)

RN 654068-75-4 ZCAPLUS

CN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[3-[(nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, (<math>\alpha Z$ )- (CA INDEX NAME)

Double bond geometry as shown.

RN 654068-76-5 ZCAPLUS

CN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, <math>(\alpha Z)-(CAINDEX NAME)$ 

RN 654068-79-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654068-81-2 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654068-83-4 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-

## (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c} O & O & (CH_2) & O & NO_2 \\ \hline O & O & \\ \hline Z & O & \\ \hline Me & Ph & \\ \hline O & O & \\ \hline \end{array}$$

RN 654068-84-5 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 654068-85-6 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

RN 654068-86-7 ZCAPLUS

CN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (<math>\alpha$ Z)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 654068-87-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (<math>\alpha$ Z)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 654068-88-9 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, ( $\alpha$ Z)-(CA INDEX NAME)

RN 654068-89-0 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, hydrochloride (1:1), ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

● HCl

RN 654068-90-3 ZCAPLUS

CN Benzeneacetic acid,  $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[3-[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester, <math>(\alpha Z)-(CA\ INDEX\ NAME)$ 

Double bond geometry as shown.

NAME)

RN 654068-95-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

RN 654068-98-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-03-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-09-7 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[[3-[[[(1,1-

dimethylethyl)dimethylsilyl]oxy]methyl]phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-10-0 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-11-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

RN 654069-15-5 ZCAPLUS

Benzeneacetic acid,  $\alpha$ -[2-[[3-(bromomethyl)benzoyl]oxy]-1-[4-CN (methylsulfonyl)phenyl]ethylidene]-, methyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:472491 ZCAPLUS

DOCUMENT NUMBER: 135:76524

TITLE: Preparation of nitrosated and

nitrosylated cyclooxygenase-2 inhibitors

INVENTOR(S): Bandarage, Ramani R.; Bandarage, Upul K.; Fang,

Xinqin; Garvey, David S.; Letts, L. Gordon; Schroeder,

Joseph D.; Tam, Sang William

PATENT ASSIGNEE(S):

Nitromed, Inc., USA PCT Int. Appl., 230 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICA	TION NO.	DATE						
WO 2001045703	A1 20010	0628 WO 2000	WO 2000-US35014							
W: AE, AG, AL,	AM, AT, AU,	AZ, BA, BB, BG	, BR, BY, BZ,	CA, CH, CN,						
CR. CII. CZ.	DE DK DM	DZ. EE. ES. FI	GB. GD. GE.	GH. GM. HR.						

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HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
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     CA 2393724
                          Α1
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     EP 1246621
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                                            EP 2000-989422
                                                                    20001222
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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                                           BR 2000-17037
     BR 2000017037
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                                20030610
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                                                                    20001222
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                                            NZ 2000-519781
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     AU 782971
                                            AU 2001-25928
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    MX 2002006312
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                                            MX 2002-6312
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                                                                    20020624
                                            ZA 2002-5707
     ZA 2002005707
                                20031111
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     US 20030220228
                                20031127
                                            US 2003-463671
                                                                    20030618
                         Α1
     US 7166618
                         В2
                                20070123
     US 20070060571
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                                20070315
                                            US 2006-599519
                                                                    20061115
     US 7432285
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     US 20090099139
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                                20090416
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PRIORITY APPLN. INFO.:
                                            US 1999-171623P
                                                                P 19991223
                                            US 2000-226085P
                                                                Ρ
                                                                    20000818
                                            US 2000-741816
                                                                A3 20001222
                                            WO 2000-US35014
                                                                W 20001222
                                            US 2003-463671
                                                                A3 20030618
                                            US 2006-599519
                                                                A3 20061115
OTHER SOURCE(S):
                         MARPAT 135:76524
     346683-81-6P 346683-83-8P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
RN
     346683-81-6 ZCAPLUS
     Benzeneacetic acid, \alpha-[2-(acetyloxy)-1-[4-
CN
     (methylsulfonyl)phenyl]ethylidene]-4-fluoro-,
     3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester,
     (\alpha Z) - (CA INDEX NAME)
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RN 346683-83-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:462317 ZCAPLUS

DOCUMENT NUMBER: 125:114294

ORIGINAL REFERENCE NO.: 125:21435a,21438a

TITLE: Preparation of stilbene derivatives useful as

cyclooxygenase-2 inhibitors

INVENTOR(S): Atkinson, Joseph G.; Wang, Zhaoyin PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.					KIND		DATE		APPLICATION NO.							DATE			
WO	9613	9613483					19960509		WO 1995-CA601							19951024				
	W:	AL,	ΑM,	ΑU,	BB,	BG,	BR,	BY,	CA,	CI	٧,	CZ,	EE,	FI,	GE,	HU,	IS,	JP,		
		KG,	KR,	KΖ,	LK,	LR,	LT,	LV,	MD,	MC	3,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,		
		RU,	SG,	SI,	SK,	TJ,	TM,	TT,	UA,	US	S,	UZ								
	RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CF	Ι,	DE,	DK,	ES,	FR,	GB,	GR,	IE,		
							SE,													
		ΝE,	SN,	TD,	TG															
CA	2200462				A1 19960509				CA 1995-2200462						19951024					
AU	9536950			A 19960523			AU 1995-36950						19951024							
AU	6889	80			В2		1998	0319												
EP	P 788476			A1 19970813			EP 1995-944787						19951024							
EP	7884	76			В1		1999	1020												
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	Я,	ΙE,	IT,	LI,	LU,	NL,	PT,	SE		
JP	1050	7765			T		1998	0728		JΡ	19	95-	5142	0 4		1	9951	024		
AT	1857	97					1999	1115		ΑT	19	95-	9447	87		1	9951	024		
ES	2139	959			Т3		2000	0216		ES	19	95-	9447	87		1	9951	024		
US	5849	943			A		1998	1215		US	19	997-	8171.	28		1	9970	407		
PRIORIT	Y APP	LN.	INFO	. :						US	19	994-	3301	72	i	A1 1	9941	027		
										WO	19	995-	CA60	1	1	W 1	9951	024		
OTHER S	HER SOURCE(S):					PAT	125:	1142	94											

OTHER SOURCE(S): 179174-84-6P

ΙT

MARPAT 125:114294

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

179174-84-6 ZCAPLUS RN

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-

> (methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

179174-89-1 179174-90-4 179174-95-9 ΙT

179175-00-9 179175-04-3 179175-09-8

179175-14-5

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

RN 179174-89-1 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(benzoyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

RN 179174-90-4 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179174-95-9 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-00-9 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

RN 179175-04-3 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[1-[4-(aminosulfonyl)phenyl]-2- (benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-09-8 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-14-5 ZCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 10:54:15 ON 17 JUN 2009)

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009

L1 STRUCTURE UPLOADED

L2 4 S SAM SSS L1 L3 84 S FULL SSS L1

FILE 'ZCAPLUS' ENTERED AT 11:14:23 ON 17 JUN 2009

E US2006-586573/APPS

L4 1 S US2006-586573/APPS

SEL RN

FILE 'REGISTRY' ENTERED AT 11:15:49 ON 17 JUN 2009

L5 34 S E1-E34 L6 4 S L3 AND L5

FILE 'ZCAPLUS' ENTERED AT 11:18:58 ON 17 JUN 2009

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L8 1 S L7 AND (NITROSATED OR NITROSYLATED)

L9 11 S L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE

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ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

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COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 67.29 277.05

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